

IN THE CLAIMS:

The text of all pending claims (including withdrawn claims) is set forth below. Cancelled and not entered claims are indicated with claim number and status only. The claims as listed below show added text with underlining and deleted text with ~~strikethrough~~. When strikethrough cannot easily be perceived, or when five or fewer characters are deleted, [[double brackets]] are used to show the deletion. The status of each claim is indicated with one of (original), (currently amended), (cancelled), (withdrawn), (new), (previously presented), or (not entered).

Please AMEND claims 5, 9, 21, and 25-27 and CANCEL claims 11 and 24 without prejudice or disclaimer in accordance with the following:

1-4. (cancelled)

5. (currently amended) A method of analyzing three-dimensional structures of a predetermined amino acid sequence probe and a protein molecule target, wherein the predetermined amino acid sequence probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the protein molecule target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

generating, by a superposition calculating unit, a combination of correspondences comprising generating ~~a~~the combination by generating a decision tree having at least one retrieval path, the decision tree being based on determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and based on minimized root mean square distance (rmsd) values between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an ~~attribute-~~rmsd value of a candidate for the combination of correspondences ~~point~~ is greater than the predetermined threshold value ~~to generate a restricted set of candidates, and determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and refining the elements of the first and second point sets based on coinciding attributes of the elements of the first and second point sets to provide a first subset and a second subset, respectively;~~

calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first subset of the first point set relating to the elements belonging to the second subset of the second point set in the generated combination of correspondence;

determining, by the superposition calculating unit, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set; and

displaying, by a graphic display unit, the three-dimensional structures of the predetermined amino acid sequence probe and the protein molecule target in an overlapped manner based on the generated combination of correspondence ~~and minimized root mean square distance values~~.

6. (previously presented) The method of claim 5, wherein the generating the combination of correspondences is based on an order relation of the elements in the first and the second point sets that are ordered.

7. (previously presented) The method of claim 5, wherein the generating the combination of correspondences is based on a proximity in a geometric relationship among a plurality of elements close to each other.

8. (cancelled)

9. (currently amended) The method of claim 5, wherein the generating the combination of correspondences is based on a condition such that ~~a~~an attribute value of a candidate for the combination of correspondence satisfies a predetermined threshold value condition.

10. (cancelled)

11. (cancelled)

12-20. (cancelled)

21. (currently amended) An apparatus for analyzing three-dimensional structures of a

predetermined amino acid sequence probe and a protein molecule target, wherein the predetermined amino acid sequence includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the protein molecule target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined amino acid sequence probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the protein molecule target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

a superposition calculating unit generating a combination of correspondence by generating a decision tree having at least one retrieval path, calculating a root mean square distance (rmsd) between the elements belonging to the first point set relating to the elements belonging to the second point set in the combination of correspondence generated, wherein the generating the combination of correspondence includes generating a~~the~~ desired combination based on determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set and based on a minimized root mean square distance values between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute-rmsd value of a ~~candidate for the combination of correspondences~~point is greater than the predetermined threshold value to generate a restricted set of candidates, and determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and refining the elements of the first and second point sets based on corresponding attributes of the elements of the first and second point sets to provide a first subset of the first point set and a second subset of the second point set, respectively; and determining, based on the generated combination of correspondence and minimizing root mean square distance values of the first subset of the first point set relating to the elements belonging to the second subset of the second point set, similar portions of the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

a graphic display unit displaying the three-dimensional structures of the first structure and the second structure in an overlapped manner based on the calculated combination of

correspondence and the minimized root mean square distance values.

22-23. (cancelled)

24. (cancelled)

25. (currently amended) A method of analyzing three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three-dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

generating, by a superposition calculating unit, a combination of correspondence by generating a decision tree having at least one retrieval path, generating a ~~desired~~the combination based on determining that a point is a candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and based on a minimized root mean square distance (rmsd) values between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute rmsd value of a ~~candidate for the combination of~~ correspondence~~point~~ is greater than the predetermined threshold value to generate a restricted set of candidates, and determining that a point is the candidate if ~~an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set~~, and refining the elements of the first and second point sets based on corresponding attributes of the elements of the first and second point sets to provide a first subset and a second subset, respectively;

calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first subset of the first point set relating to the elements belonging to the second subset of the second point set in the generated combination of correspondence;

determining, by the superposition calculating unit, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the

three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

displaying, by a graphic display unit, the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on the generated combination of correspondence and minimized root mean square distance values.

26. (currently amended) A computer-readable medium containing computer-readable instructions to analyze three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, the computer-readable instructions comprising:

generating a combination of correspondence comprising generating a ~~desired~~ the combination based on determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and based on a minimized root mean square distance (rmsd) values between the first and second point sets, setting a predetermined threshold value and pruning a retrieval path if an attribute ~~rmsd~~ value of a ~~candidate for the combination of correspondences~~ point is greater than the predetermined threshold value to generate a restricted set of candidates, and determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set, and refining the elements of the first and second point sets based on corresponding attributes of the elements of the first and second point sets to provide a first subset and a second subset, respectively;

calculating, by the superposition calculating unit, a root mean square distance between the elements belonging to the first subset of the first point set relating to the second subset of

the elements belonging to the second point set in the generated combination of correspondence; determining, based on the generated combination of correspondence and minimizing root mean square distance values, similar portions of the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set; and

causing to be displayed, on a display, the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on the generated combination of correspondence and minimized root mean square distance values.

27. (currently amended) An apparatus for analyzing three-dimensional structures of a predetermined molecular structure probe and a molecular structure target, wherein the predetermined molecular structure probe includes a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and the molecular structure target includes a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, to determine a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second point set, comprising:

a database having data having stored therein that includes a plurality of three-dimensional molecular structures of substances representing a plurality of predetermined molecular structure probes, each having a first structure expressed by three-dimensional coordinates of elements belonging to a first point set;

a data input unit that reads the data and an input command from a user selecting a molecular structure target that includes the second structure expressed by three-dimensional coordinates of elements belonging to the second point set;

a superposition calculation unit that generates a combination of correspondence comprising generating ~~a desired~~the combination based on determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set to provide a first subset of the first point set and a second subset of the second point set, and based on a minimized root mean square distance (rmsd) values between the first and second point sets,

setting a predetermined threshold value and pruning a retrieval path if an attribute rmsd value of a candidate for the combination of correspondences point is greater than the predetermined threshold value, and determining that a point is the candidate if an attribute of an element of the first point set includes a type of an atom, an atomic group, a molecule, a hydrophilic property, a hydrophobic property, or a positive or negative charge that coincides with an attribute of an element of the second point set to provide a first subset of the first point set and a second subset of the second point set, respectively, determines a degree of similarity between the three dimensional structure of the predetermined molecular structure probe represented by the three-dimensional coordinates of the elements belonging to the first subset of the first point set and the three-dimensional structure of the molecular structure target represented by the three-dimensional coordinates of elements belonging to the second subset of the second point set, and superposes a three-dimensional molecular structure of a predetermined molecular structure probe read from the database with a three-dimensional molecular structure target in accordance with the desired combination and having minimized root mean square distance values; and

a graphic display unit that displays the three-dimensional structures of the predetermined molecular structure probe and the molecular structure target in an overlapped manner based on the calculations of the superposition calculation unit.